A Percolation Model of Diagenesis

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The restructuring process of diagenesis in the sedimentary rocks is studied using a percolation type model. The cementation and dissolution processes are modeled by the culling of occupied sites in rarefied and growth of vacant sites in dense environments. Starting from sub-critical states of ordinary percolation the system evolves under the diagenetic rules to critical percolation configurations. Our numerical simulation results in two dimensions indicate that the stable configuration has the same critical behaviour as the ordinary percolation.

Key Words: Diagenesis, Porosity, Percolation, Scaling

I. INTRODUCTION

Rocks in general, particularly sedimentary rocks e.g. sandstones, limestones etc., have porous structures. Typically such a pore space is a highly branched and interconnected network. Study of the pore structure of sedimentary rocks is important from a practical point of view, in problems such as oil-exploration, ground water flow, spread of pollutants etc.

An interesting property of these rocks is that they appear not to have a finite percolation threshold [1]. These rock materials are conducting when the pore space is filled with saline water. It has been observed that these rock samples show finite conductivity even when the porosity is less than one percent. This implies that a connected network of pores exists in the macroscopic length scale, even when the porosity i.e., the volume fraction of the void space is very little.

Several empirical laws reflect this property. Archie's law [2] connects the conductivity $\sigma(\phi)$ and the porosity ϕ in the following way:

$$\sigma(\phi)/\sigma_w = a\phi^z \tag{1}$$

Here, σ_w is the conductivity of water, $a \sim 1$ is an empirical parameter and $z \sim 2$ is a non-universal exponent that depends on characteristics of the rock structure. This law suggests that a finite conductivity exists even in the limit of $\phi \to 0$ and therefore the percolation threshold is zero.

The permeability $K(\phi)$ of the rock structure is related to the porosity ϕ through a similar power law, known as Kozeny equation [3]:

$$K(\phi) = c\phi^{z'}/S_o^2 \tag{2}$$

where, $z' \approx 3$, S_o is the specific surface area and c is an empirical constant. This equation also suggests the global connectivity of the pore space is maintained in the $\phi \to 0$ limit.

A physical process which is responsible for achieving a connected pore structure at very low porosities is known as "diagenesis". Diagenesis is a complex restructuring process by which granular systems evolve in geological time scales from unconsolidated, high-porosity packings toward more consolidated, less porous structures. Formation of sedimentary rocks starts with deposition of sand grains under water or in air [4–6]. Initially this gives an unconsolidated and highly porous $\sim 40-50\%$ sediment. Sedimentation is followed by compaction under pressure and diagenesis, before the consolidated sandstone is formed from the loosely packed sediment [7]. Diagenesis may reduce porosity by an order of magnitude and permeability by as much as four orders of magnitude [4].

The final characteristic of the pore network depends strongly on the diagenetic process. Sandstones are usually formed under water, which contains dissolved salts. Depending on the nature of the pore-filling fluids, salts may be deposited as crystallites in the crevices or along walls of the rock structure, a process called "cementation". Otherwise, portions of the existing solid structure may get eroded or dissolved out in a "dissolution" process. The former decreases the porosity of the rock while the latter increases porosity. The two processes may take place simultaneously. The details of the chemical nature of the solid and pore filling fluid determines whether diagenesis leads finally to a stable structure, or to a continuously developing structure eventually giving rise to caverns of macroscopic size.

Sahimi had classified the theoretical studies of modeling diagenesis in two ways [6]. The approach of "chemical modeling" relies on solving continuum equations of transport and reactions ignoring the morphology of the pore space. The second approach is "geometrical modeling" in which the reaction kinetics and mass transfer are ignored. These models start with geometrical descriptions of initial unconsolidated pore space which evolves under simple rules leading to reduction of porosities but maintaining the connectivity. For example the model of Wong et. al. [8] starts with a regular lattice in which each bond is a fluid filled cylindrical tube of uniform radius and conductivity. This system evolves to a random resistor network through a random bond-shrinkage

mechanism where randomly selected bonds of the network shrinks its radius by a constant factor. This model maintains global connectivity even in the limit of $\phi \to 0$ and reproduces power law behaviour as in Archie's law. A second model of Roberts and Schwartz [9] starts with a Bernal distribution of dense random spheres of equal radii modeling grains. These spheres grow in unison and the pore space, i.e. the space not covered by the spheres shrinks its volume. This model gives a low but non-zero percolation threshold $\phi_c \approx 3.5\%$. The bimodal ballistic deposition model (BBDM) [10] tries to represent the deposition realistically, but does not address the problem of diagenesis.

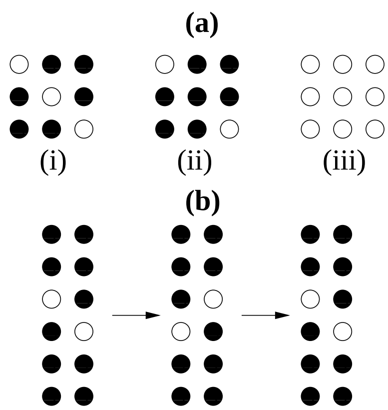

FIG. 1. (a) On an initial configuration as in (i) if the central site is first updated one gets the SC in (ii). However if the sequential updating rule (I) (see text) is used one gets the SC as in (iii). (b) In parallel updating this configuration is locked in a period of cycle 2.

In our model, we do not take into account the effect of chemical reactions explicitly, so this is also a geometrical modeling of diagenesis. We try to simulate the restructuring as it may actually occur in porous rocks due to fluid flow. Isolated projected grains on a wall are smoothed out modeling dissolution, and a gap or cul-de-sac in a solid is filled by deposition modeling cementation. The restructuring involves two processes. Growth of the solid phase at sites with a relatively larger number of occupied nearest neighbours, to represent cementation, and removal or culling of occupied sites which are isolated, or have too few nearest neighbours, to represent dissolution. This algorithm is a stabilizing process leading to a stable structure after several time steps. It may be regarded as a self-organizing process as discussed recently by several authors [11,12].

Before proposing our model, we briefly describe two other physical situations which are closely related to our study on diagenesis. In the Bootstrap percolation model (BPM) occupied sites of a randomly occupied regular lattice with certain probability having fewer than certain number of occupied neighbours are successively removed [13–18]. On repeated application of this process the system reaches a stable configuration where no further sites can be culled. The threshold value of the probability at which the stable configuration is percolating is calculated.

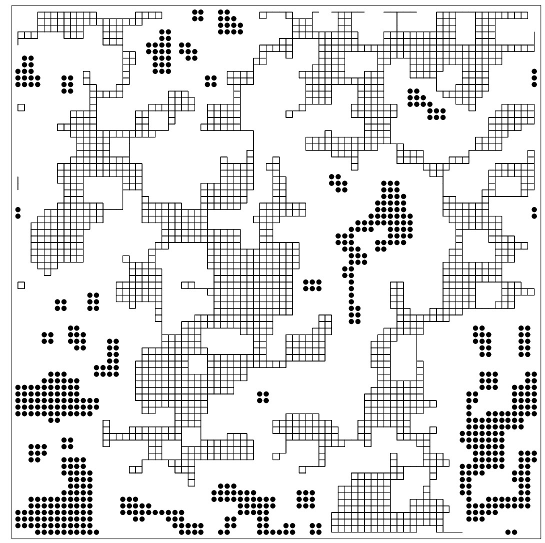

FIG. 2. A stable configuration of the diagenetic percolation for a system of size $L = 80$ and with m=2. Sites on the "infinite" incipient cluster are joined by lines and sites on the isolated clusters are shown by filled circles.

Secondly, consider the nearest neighbour Ising model at the zero temperature with Glauber spin-flip dynamics in the absence of an external magnetic field. Here the direction of a spin follows the direction of the majority of the neighbouring spins. In the case when there are equal number of up and down spins in the neighbourhood, a spin decides its direction with equal probability. Recently it has been observed in [19] that starting from an arbitrary random initial configuration of spins this system does not reach the global ground states where all spins are either up or down but arrive at a frozen two-stripe state in a finite fraction of cases [19].

In next section we describe our model and also the updating rules used. Section III describes our results and we summarize in section IV.

II. MODEL

In our model, the sites of a regular lattice are randomly occupied ($s_i = 1$) with a probability p representing pores and are kept vacant ($s_i = 0$) with a probability $1 - p$ representing solid grains. This configuration therefore models the initial unconsolidated porous structure with porosity $\phi(p) = p$.

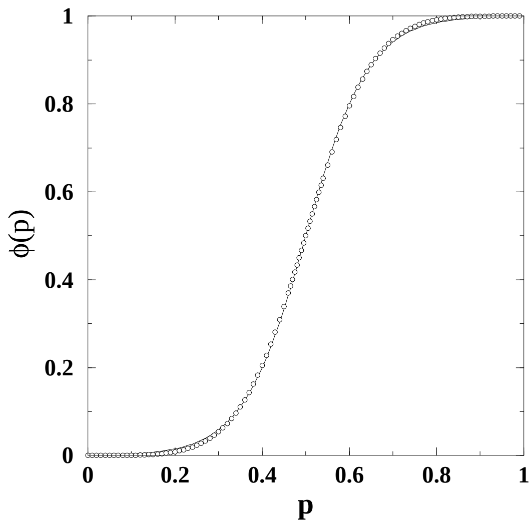

FIG. 3. The porosity $\phi(p)$ as a function of the initial occupation probability p for a system size $L = 64$. The continuous curve is a fit to the data having the form given in Eqn. 1.

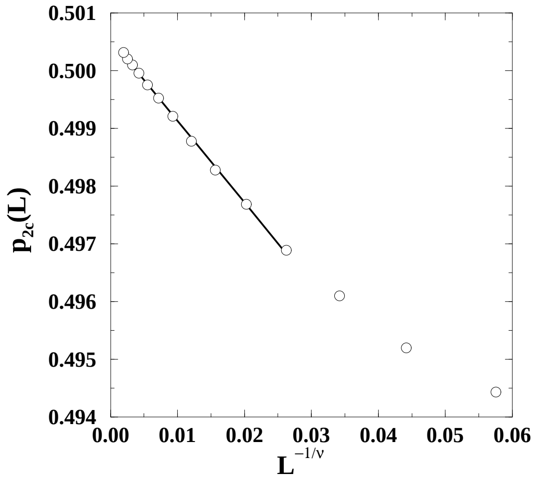

FIG. 4. The plot of the percolation thresholds $p_{2c}(L)$ for $m = 2$ for finite system sizes L as a function of $L^{-1/\nu}$. Using $\nu = 4/3$, the correlation length exponent for ordinary percolation, we get the linear fit for large L values. The extrapolated value for p_{2c} is 0.5005.

The occupation status of a site i depends on its neighbour number i.e., the number of occupied neighbours $n_i = \Sigma_j s^i_j$ where, s^i_j is the occupation of the j-th neighbour of the site i. All sites of the lattice are sequentially updated according to the following diagenetic conditions: (i) *Culling condition*: Occupied sites having fewer than m occupied nearest neighbours are vacated i.e., $s_i \to 0$ if $n_i < m$ (ii) the sites with exactly m occupied neighbours remain unaltered i.e., $s_i \to s_i$ if $n_i = m$ and (iii) *Growing condition*: Vacant sites having more than m occupied nearest neighbours are occupied i.e., $s_i \to 1$ if $n_i > m$.

Starting from the initial configuration the system evolves in different time steps following these rules. One time step consists of update attempts of all the lattice sites. One sweep of the lattice results in another occupied configuration which is again updated by the same rules. This process is continued till the system reaches a stable configuration (SC) where no further site changes its occupied or vacant status. In general the SC may have many clusters of occupied sites. However, there exists a percolation threshold p_{mc} of p depending on the value of m so that the SC must have a spanning ("infinite") cluster of occupied sites for $p > p_{mc}$ in an infinitely large system.

Like the cellular automata models, the updating of the sites is important in our problem. Three possible sequential updating procedures are as follows: (I) Sites are labeled from 1 to L^2 from left to right along a row and from the first row to the last row. (II) Only sites with $n_i \neq m$ are randomly selected and updated. (III) The lattice is divided into odd and even sub-lattices and are updated alternately but sequentially as in (I).

For BPM, it has been shown in [17] that the SC is independent of the updating sequence. In contrast here the SC does depend on the updating sequence because culling at one site may inhibit growth at a neigbouring site and vice versa. This is seen by considering the neighbour numbers at all sites of the lattice. When $n_i < m$ the culling of the site i reduces the neighbour numbers at all neighbouring sites by one i.e., $n_j \to n_j - 1$ where as the growth at i enhances the neighbour numbers at all neighbouring sites i.e., $n_j \to n_j + 1$. Therefore the culling at one site may suppress the growth at a neighbouring site and vice versa. In Fig. 1(a) we show an example where two different updating sequences lead to different SCs. On the other hand, in a fully parallel update all sites of the lattice are updated simultaneously at a certain time depending on the configuration at the previous time. There may arise some situations as shown in Fig. 1(b) where a particular cluster of sites never goes to a stable configuration but takes two different configurations alternately in a two cycle periodic state.

A cluster of occupied sites, in which every site has at least m occupied neighbours, is called an m-cluster [14]. Imposition of our diagenetic rules imply that the surviving clusters in SC must be m clusters. An isolated cluster of occupied sites in a d-dimensional hypercubic lattice always has some convex corners on the surface with d neighbours. Therefore in the case when $m \geq d+1$ these sites are always unstable and therefore, the SC cannot have any finite cluster and has only one infinite m-cluster. A SC at the percolation threshold for $m = 2$ is shown in Fig. 2, the smallest isolated clusters being of size 4.

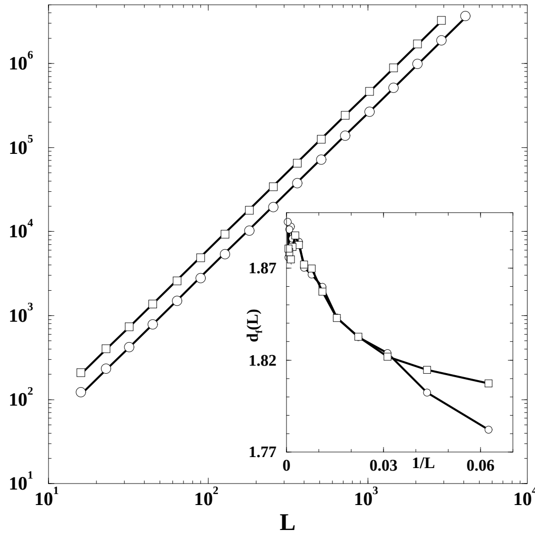

FIG. 5. The average mass of the infinite cluster S^1_∞ (circle) and the largest cluster $2S^2_\infty$ (square) at the diagenetic percolation threshold $p_{2c}(L)$ are plotted with the system size L. Average fractal dimension is obtained from the linear fits shown by continuous lines. The inset shows the variations of the local slopes $d_f(L)$ and we conclude a value of the fractal dimension $d_f = 1.89 \pm 0.02$.

III. RESULTS

The average fraction $\phi(p)$ of the occupied sites in the SC is defined as the porosity of this model. We measure this porosity as a function of the probability p and this variation is plotted in Fig. 3. We find no trace of any system size dependence on this variation. A functional form like

$$\phi(p) = 1/[1 + \exp((1/2 - p)/\Delta p)] \tag{3}$$

fits very well to this data with a value of $\Delta p = 0.072$. The data as well as the fit are very well consistent to $\phi(1/2) = 1/2$ as expected from the symmetry of occupied and vacant sites. Compared to the porosity $\phi(p) = p$ in the initial random distribution of occupied and vacant sites, the porosity in SC is reduced by an order of magnitude when $p < 0.35$. We consider this as the reflection of the diagenesis process in nature observed in our model.

Like BPM, the culling condition in our model does not contribute to change the percolation threshold for $m \leq 2$. For example, nothing is culled for m=0, isolated sites are culled for $m = 1$ and the dangling chain of sites are culled for $m = 2$. Since the connectivity of the system is not affected by these culling processes, the difference between p_{mc} and $p_c(ord)$ is due to the growing condition for $m \leq 2$, where $p_c(ord)$ is the ordinary percolation threshold. For p values very close to $p_c(ord)$ but smaller than it, there may be some initial configurations which are not connected because of the presence of only few vacant sites. If these sites have more than m occupied neighbours they will now be occupied ensuring the global connectivity of the system. Therefore it is expected that the $p_{mc} \leq p_c(ord)$ for $m \leq 2$ on an arbitrary lattice. Therefore as the growth rule helps in attaining a connectivity in the system we expect $p_{mc} \leq p_c(BPM)$ for any arbitrary lattice and for any arbitrary value of m.

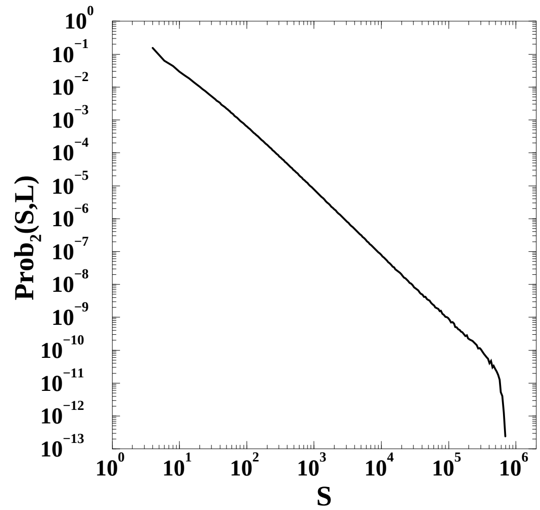

FIG. 6. The distribution of the cluster sizes of the stable configuration at the percolation threshold of a lattice of size $L = 2048$ and with $m = 2$.

The percolation threshold p_{mc} is the minimum value of the probability p beyond which an infinite cluster of occupied sites exists with probability one in the SC on an infinitely large system. However, for systems of finite size this threshold $p_{mc}(L)$ depends on the system size. The correlation function $g(r)$ for the percolation problem is defined as the probability that a site at a distance r apart from an occupied site belongs to the same cluster. For $p < p_{mc}$ the correlation function is expected to decay exponentially as $g(r) \sim \exp(-r/\xi)$ where the correlation length ξ, a measure of the typical cluster diameter, diverges as $\xi \sim (p_{mc} - p)^{-\nu}$ where, ν is the correlation length exponent for the diagenetic percolation.

We use the standard method of estimating the value of the percolation threshold. Using a specific sequence of random numbers, the lattice is filled at some high value of $p = p_{hi}$ such that its SC has an infinite cluster. Similarly using the same sequence of random numbers, the lattice is filled at some low value of $p = p_{lo}$ so that its corresponding SC does not have an infinite cluster. It is then similarly tried at a $p = (p_{hi} + p_{lo})/2$. If its SC is connecting then p_{hi} is equated to p, otherwise p_{lo} is equated to p. This process is continued till the difference

$(p_{hi} - p_{lo})$ is less than a certain pre-assigned small number $\epsilon = 10^{-5}$ when $p(seq) = (p_{hi} + p_{lo})/2$ is taken for the percolation threshold for this particular sequence of random numbers. Averaging over the $p(seq)$ values for a large number of independent random number sequences one obtains the estimate for $p_{mc}(L)$.

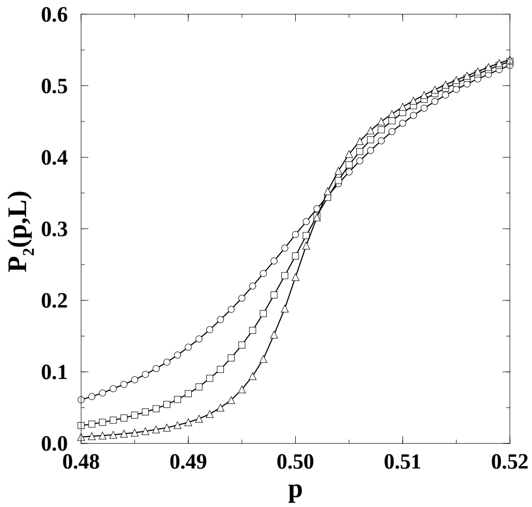

FIG. 7. The plot of the percolation probability $P_2(p, L)$ for $m = 2$ of the diagenetic percolation for three different system sizes $L = 256$ (circle), 512 (square) and 1024 (triangle).

In this process, we tune the probability p to the percolation threshold $p_{mc}(L)$ on a system of size L so that the correlation length is of the same order as the system size. Therefore for $m = 2$, $L \sim (p_{2c} - p_{2c}(L))^{-\nu}$ which implies

$$p_{2c}(L) = p_{2c} + A.L^{-1/\nu} \tag{4}$$

We plot $p_{2c}(L)$ in Fig. 4 with $L^{-1/\nu}$ and we try $\nu = 4/3$, the value for the correlation length exponent in the ordinary percolation. We observe a linear variation for large L values. On extrapolation, we find a slightly larger value of $p_{2c} = 0.5005(2)$ for sequential updating of type (I) as stated above. The $p_{mc}(L)$ values for L=2048, 2896 and 4096 are found larger than 1/2. For the random and sublattice sequential updatings the p_{2c} values are 0.5013 and 0.5009 respectively. These values should compared to the ordinary percolation threshold of 0.592746 on square lattice [20].

Since $m = 2$ is the middle point of the five possible values of the neighbour numbers on a square lattice (i.e. from 0 to 4) and due to the equivalence of vacant and occupied sites, it may be expected that p_{2c} should be exactly equal to 1/2. However, we argue that the value of p_{2c} very close to 1/2 is actually accidental and there is no reason why it should be 1/2. We believe that first appearnce of the global connectivity through occupied sites determining the percolation threshold is a very special situation and since we want this connectivity through the occupied sites we break the symmetry between the occupied and vacant sites. An estimate of the similar percolation threshold for $m = 3$ on a simple cubic lattice gives a value much lower than 1/2. However, for $m = 3$ on the triangular lattice the value of the percolation threshold is obtained as 0.50 ± 0.01.

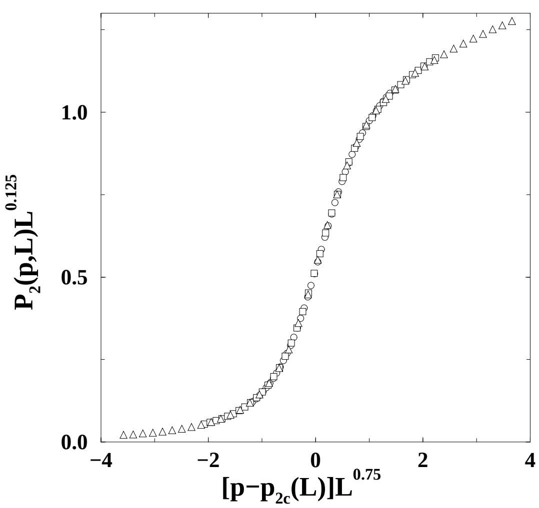

FIG. 8. The diagenetic percolation probability $P_2(p, L)$ as shown in the previous figure for different system sizes are scaled as $P_2(p, L)L^{\beta/\nu}$ with $[p - p_{2c}(L)]L^{1/\nu}$. The collapse is obtained using ν=4/3 and β/ν =0.125.

The $p(seq)$ values corresponding to different sequences of random numbers are spread around their mean value $p_{mc}(L)$. The root mean square deviation from the average value

$$\Delta(L) = (< p(seq)^2 > -[p_{mc}(L)]^2)^{1/2} \tag{5}$$

is supposed to have a dependence on the system size L as: $\Delta(L) \sim L^{-1/\nu}$. Plotting $\Delta(L)$ vs. L for $m = 2$ on a double logarithmic scale which fits nicely to a straight line gives a value for the correlation length exponent $\nu = 1.35(2)$.

The fractal dimension d_f of the "infinite" incipient cluster (IIC) of the SC exactly at the percolation threshold is also calculated. A large number of SCs are generated at $p = p_{2c}$. The average size S_∞ of the IIC is calculated in two ways: (i) Average size $S^1_\infty(L)$ of the infinite clusters is measured over the spanning SCs only (ii) Average size $S^2_\infty(L)$ of the largest cluster is calculated over all SCs. Using the definition of percolation probability as defined below, $S^2_\infty(L) = L^2 P_2(p_{2c}(L), L)$. Both measures of the IIC are expected to give the fractal dimension: $S^{1/2}_\infty(L) \sim L^{d_f}$. In Fig. 5 we plot both $S^1_\infty(L)$ and $2S^2_\infty(L)$ with L on a double logarithmic scale for the

system sizes varying from 16 to 4096. The average slopes are 1.863 and 1.860 for $S^1_\infty(L)$ and $S^2_\infty(L)$ respectively. Further, we plot the local slopes $d_f(L)$ with $1/L$ in the inset of Fig. 5. After considerable variation over the small systems the fractal dimension seems to converge at 1.89 ± 0.02 for the large system sizes compared to 91/48 of the ordinary percolation [1].

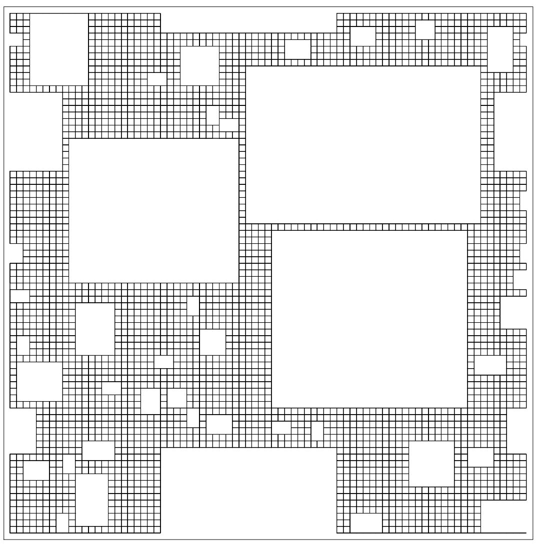

FIG. 9. A stable configuration (SC) at the percolation threshold for a system size of $L = 80$ and with m=3. Sites on the "infinite" incipient cluster are joined by lines.

The cluster size distribution of occupied sites on the SCs are also measured at the percolation threshold. We define $\mathrm{Prob}_2(S, L)$ as the probability of a cluster of S occupied sites on a SC of a system of size L with $m = 2$. We start from many independent configurations at $p_{2c}(L) \approx 0.5001$ for $L = 2048$. These are sub-critical configurations for the ordinary percolation. We measure the $\mathrm{Prob}_2(S, L)$ at each time step and keep track of how this distribution changes from the initial exponential distribution to the power law distribution as shown in Fig. 6. We notice that at very short times of the order of 1, the distribution takes the form of the steady state distribution. In this distribution we do not include the "infinite" cluster spanning the system. As expected the distribution appears to be a power law: $\mathrm{Prob}_2(S, L) \sim S^{-\tau}$ where $\tau = 2.02 \pm 0.06$ is obtained compared to 187/91 for the ordinary percolation [1].

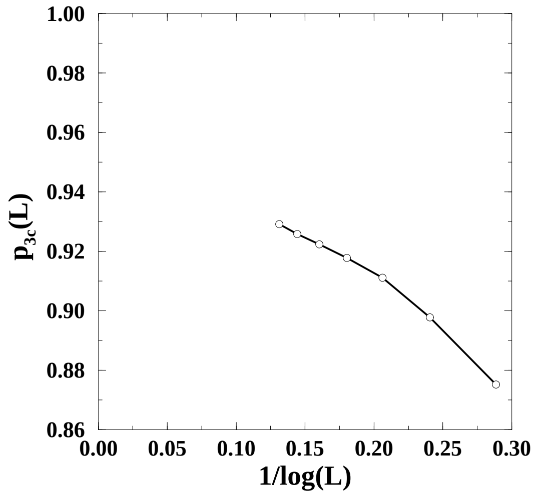

FIG. 10. Plot of $p_{3c}(L)$ with $1/\log(L)$ which on extrapolation to $L \to \infty$ gives $p_{3c} = 0.96 \pm 0.01$.

The order parameter is the percolation probability $P_m(p)$ that is the average fraction of sites on the largest occupied cluster in the SC. For finite systems it is denoted by $P_m(p, L)$. Variation of the percolation probability is shown in Fig. 7 and it varies as:

$$P_m(p, L) \sim [p - p_{mc}(L)]^\beta \tag{6}$$

This variation is true in the limit of $L \to \infty$. For finite systems however, according to the scaling theory [1], the scaling variable should be L/ξ, where the correlation length is defined as $\xi = [p - p_{mc}(L)]^{-\nu}$. Therefore for a finite system of size L the variation of percolation probability should be:

$$P_m(p, L) = L^{-\beta/\nu} F[(p - p_{mc}(L))L^{1/\nu}] \tag{7}$$

where, the scaling function $F(x) \to x^\beta$ for large L. We show the collapse of the data in Fig. 8 using this scaling formulation. We again try $\nu = 4/3$ and then obtain a value of $\beta/\nu = 0.125$ for the data collapse, giving $\beta = 0.166$ compared to 5/36 for the ordinary percolation [1].

Next we studied the case of m=3 on the square lattice. In this case the SC can only be completely vacant or it can have only one infinite cluster but cannot have isolated clusters. Since in general there will always be some sites which have less than 3 occupied neighbours on the surface of an isolated cluster, these sites will be unstable under the diagenetic rules and the cluster will therefore cannot survive in SC. In Fig. 9 we show the picture of a SC for m=3. It is a simple spanning cluster having many rectangular holes as in BPM [16]. The percolation threshold $p_{3c}(L)$ also has L dependence and on extrapolation with $1/\log(L)$ (as was done in BPM) we get $p_{3c} = 0.96 \pm 0.01$ (Fig. 10).

IV. SUMMARY

The restructuring process of diagenesis in sedimentary rocks involving cementation and dissolution has been studied by a percolation model. Simulations on a square lattice shows that the porosity is highly reduced due to restructuring as is observed in rocks. We also observe that starting from the sub-critical configurations of ordinary percolation at a certain threshold value p_{2c} of the pore probability the system evolves to a globally connected porous space at the stable state. This configuration is critical since it shows long range correlations. Our numerical results give strong indications that the stable states in this model have the same critical behaviour as that of ordinary percolation. We view the dynamics under diagenetic rules as a self-organizing dynamics in a limited sense since one has to tune p to arrive at a specific sub-critical configuration at p_{2c} so that it organizes to show criticality in the stable state.

After completion of a draft of this manuscript we were informed by the editor that a spin model on a square lattice where each spin ± 1 was flipped only when more than half of its four neighbours point into the opposite direction was studied in [21]. Using a much bigger system size ($L \approx 7 \times 10^5$) compared to what we used a percolation threshold of 0.5007 ± 0.0001 was estimated which is consistent with our results.

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